# EXAFS, X-ray Diffraction and Neutron Diffraction Study of the Heusler Alloy Co<sub>2</sub>MnSi

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Magnetoelectronics is an emerging field of electronics in which electron spin is used to control the properties of magnetic devices. More specifically, these devices exploit the imbalance of spin-up and spin-down conduction electrons in ferromagnetic materials. Band structure theory predicts that Heusler alloys, which are either  $Co_2MnSi$  or  $Co_2MnGe$ , have a complete spin imbalance in the conduction band. But the actual spin imbalance in bulk and thin film samples does not exceed 60, which might be explained by the swapping of lattice positions between cobalt and nickel atoms. We have used synchrotron and neutron techniques to confirm that extensive site-swapping occurs in Heusler alloys.

Magnetoelectronic devices have been proposed for a wide variety of applications, including magnetic recording, magnetic field sensors, and nonvolatile memory. The magnetoelectronic devices with the greatest economic impact have been hard disk read heads, which read signals encoded on a magnetic disk or tape. These read heads exploit the giant magnetoresistance (GMR) effect, which is the change in the electrical resistance of a material when it is subject to the application of a magnetic field.

A GMR device consists of ferromagnetic layers separated by a metallic layer, as shown in **Figure 1**. The resistance of the device varies according to how the two ferromagnetic layers are aligned with each other. In the low resistance state, the magnetic moments of the ferromagnetic layers are in the same direction and electron transport through the sample is enhanced because a spin-up transport electron in one ferromagnetic layer is more likely to find a same-spin state to scatter into in the other ferromagnetic layer. In the high resistance state, the two ferromagnetic layers are anti-aligned and electron transport is diminished.

A magnetic storage medium stores bits as magnetic grains whose spins point in opposite directions. So, as the read head passes over the medium, the spins of the bottom layer of the read head aligns to the spins of the magnetic grains, changing their resistance and thus reading the bits in the magnetic grains.

Currently, GMR read heads are made of ferromagnets composed of cobalt, nickel, iron, or an alloy. The read heads' efficiency is limited by the relatively small spin imbalance of 40 percent. With 100 percent spin imbalance – as predicted by band theory – Heusler alloys would be attractive candidates for future GMR devices that would be smaller and would feature an increased surface density. In practice, Heuslers have spin imbalances of around 55 percent.

Band theory predicts that this imbalance would be reduced if the manganese and cobalt atoms swapped their lattice positions (**Figure 2**), an effect also called anti-site disorder. Using neutron diffraction on bulk



Authors (from left): Bruce Ravel and Marc Raphael

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Co<sub>2</sub>MnSi, we found that about 15 percent of the manganese sites are occupied by cobalt. But neutron diffraction is impractical for the small sample volumes required for GMR devices. So we turned to synchrotron techniques to measure the anti-site disorder.

We used a technique called extended x-ray absorption fine structure spectroscopy (EXAFS) at NSLS beamlines X23B and X23A2 on powdered and thin film samples of Co<sub>2</sub>MnSi. We found that about 15 percent of manganese sites are occupied by cobalt.

Because the photoelectron scattering amplitudes of cobalt and manganese are so similar, the anti-site disorder is measured with very poor precision by EXAFS. So we next turned to anomalous x-ray diffraction, and we were able to measure anti-site disorder in Heusler alloys in sample volumes comparable to those found in magnetoelectronic devices.

By using synchrotron measurement techniques, we sccessfully characterized a dominant form of disorder that limits the application of Heusler alloys to GMR devices.

## Additional Publication:

B. Ravel et al. "Atomic disorder in Heusler Co<sub>2</sub>MnGe measured by anomalous x-ray diffraction," *Appl. Phys. Letts.*, **81**, 15, 2812 (2002).

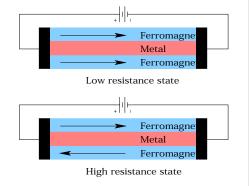


Figure 1. A giant resistive read head used in magnetic storage media consists of two ferromagnetic layers separated by a metallic layer. When the spins of the two ferromagnets are parallel (top), conduction electrons can easily scatter through the heterostructure, resulting in a low resistance. When the spins are anti-parallel, the resistance is high.

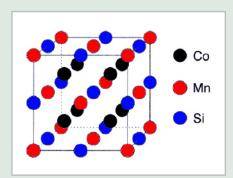


Figure 2. Crystal structure of the Heusler alloy Co<sub>2</sub>MnSi.